

Kinetics of local "magnetic" moment and non-stationary spin-polarized current in the single impurity Anderson-model

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We perform theoretical investigation of the localized state dynamics in the presence of interaction with the reservoir and Coulomb correlations. We analyze kinetic equations for electron occupation numbers with different spins taking into account high order correlation functions for the localized electrons. We reveal that in the stationary state electron occupation numbers with the opposite spins always have the same value - the stationary state is a "paramagnetic" one. "Magnetic" properties can appear only in the non-stationary characteristics of the single-impurity Anderson model and in the dynamics of the localized electrons second order correlation functions. We found, that for deep energy levels and strong Coulomb correlations, relaxation time for initial "magnetic" state can be several orders larger than for "paramagnetic" one. So, long-living "magnetic" moment can exist in the system. We also found non-stationary spin polarized currents flowing in opposite directions for the different spins in the particular time interval.

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I. INTRODUCTION

The creation, diagnostics and controlled manipulation of charge and spin states of the impurity atoms or quantum dots (QDs) is one of the most important problems in nano-electronics now a days^{1,2,3,4,5}. Modern ultra small size electronic devices design with a given set of electronic transport parameters requires careful analysis of non-stationary effects, transient processes and time evolution of electronic states prepared at the initial time moment^{6,7,8,9,11,12,13}. So, it is necessary to investigate the time dependent dynamics of initial spin and charge configurations of correlated impurity or QD. Moreover, the characteristics of stationary state of single impurity interacting with the reservoir in the presence of strong Coulomb correlations are not completely understood^{10,14,15,16}.

The possibility of the localized non-zero magnetic moment existence on the single impurity or single-level QD, interacting with the reservoir, in the absence of external magnetic field is still unclear. Results obtained in the mean-field approximation for the one-level Anderson model allowing the presence of magnetic state (electron occupation numbers with opposite spins have different values) for the single impurity with strong on-site Coulomb repulsion seems to be rather questionable.

The single-impurity Anderson model for a long time served as a basic one for the understanding of the nature of local magnetic moments in solids^{17,18}. For a single partly occupied impurity state, the correlation energy acts to prevent the appearance of a non-vanishing ground-state spin, while in low-density limit the Hartree-Fock theory still predicts a non-zero magnetic moment over a range of parameters¹⁹. As it was argued in¹⁹ the magnetism is possible only when several degenerate orbitals are present on the impurity in the Anderson model.

Local moment approach to the Anderson model has been applied for the case of half-filling in²⁰.

The most adequate approach for this problem analysis is based on the non-stationary kinetic equations for localized electron occupation numbers and their correlation functions, taking into account all high-order correlation functions for the localized electrons. The simplest way to obtain the system of kinetic equations is the Heisenberg approach. These equations can be also obtained by means of Keldysh diagram technique, but it is more cumbersome procedure²¹.

In this paper we analyze the localized state dynamics in the presence of interaction with the reservoir and Coulomb correlations by means of kinetic equations for electron occupation numbers with the different spins and second order correlation functions of the localized electrons. We demonstrate that "magnetic" state can be distinguished from the "paramagnetic" one by means of the analysis of the non-stationary characteristics and dynamics of second order correlation functions.

II. THEORETICAL MODEL AND MAIN RESULTS

We consider non-stationary processes in the system of the single-level impurity coupled to an electronic reservoir with Coulomb interaction of the localized electrons. The model Hamiltonian has the form:

$$\hat{H} = \sum_{\sigma} \varepsilon_1 \hat{n}_{1\sigma} + \sum_{k\sigma} \varepsilon_k \hat{c}_{k\sigma}^{\dagger} \hat{c}_{k\sigma} + U \hat{n}_{1\sigma} \hat{n}_{1-\sigma} + \sum_{k\sigma} t_k (\hat{c}_{k\sigma}^{\dagger} \hat{c}_{1\sigma} + \hat{c}_{1\sigma}^{\dagger} \hat{c}_{k\sigma}). \quad (1)$$

Index k labels continuous spectrum states in the lead,

t_k - tunneling transfer amplitude between the continuous spectrum states and localized state with the energy ε_1 which is considered to be independent of momentum and spin. Operators \hat{c}_k^+/\hat{c}_k correspond to the electrons creation/annihilation in the continuous spectrum states k . $\hat{n}_{1\sigma(-\sigma)} = \hat{c}_{1\sigma(-\sigma)}^+ \hat{c}_{1\sigma(-\sigma)}$ -localized state electron occupation numbers, where operator $\hat{c}_{1\sigma(-\sigma)}$ destroys electron with spin $\sigma(-\sigma)$ on the energy level ε_1 . U is the on-site Coulomb repulsion for the double occupation of the localized state.

Our investigations deal with the low temperature regime when Fermi level is well defined and the temperature is much lower than all the typical energy scales in the system. Consequently the distribution function of electrons in the leads (band electrons) is close to the Fermi step.

Let us consider $\hbar = 1$ elsewhere, so the motion equation for the electron operators products $\hat{c}_{1\sigma}^+ \hat{c}_{1\sigma}$, $\hat{c}_{1\sigma}^+ \hat{c}_{k\sigma}$ and $\hat{c}_{k'\sigma}^+ \hat{c}_{k\sigma}$ can be written as:

$$\begin{aligned} i \frac{\partial \hat{c}_{1\sigma}^+ \hat{c}_{1\sigma}}{\partial t} &= - \sum_{k,\sigma} t_k \cdot (\hat{c}_{k\sigma}^+ \hat{c}_{1\sigma} - \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma}), \\ i \frac{\partial \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma}}{\partial t} &= -(\varepsilon_1 - \varepsilon_k) \cdot \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma} - U \hat{n}_{1-\sigma} \cdot \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma} + \\ &+ t_k \cdot (\hat{n}_{1\sigma} - \hat{n}_{k\sigma}) - \sum_{k' \neq k} t_{k'} \hat{c}_{k'\sigma}^+ \hat{c}_{k\sigma} \end{aligned} \quad (2)$$

and

$$\begin{aligned} i \frac{\partial \hat{c}_{k'\sigma}^+ \hat{c}_{k\sigma}}{\partial t} &= -(\varepsilon_{k'} - \varepsilon_k) \cdot \hat{c}_{k'\sigma}^+ \hat{c}_{k\sigma} - \\ &- t_{k'} \cdot \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma} + t_k \cdot \hat{c}_{k'\sigma}^+ \hat{c}_{1\sigma}, \end{aligned} \quad (3)$$

where $\hat{n}_k = \hat{c}_{k\sigma}^+ \hat{c}_{k\sigma}$ is an occupation operator for the electrons in the reservoir. From Eq.(3) one can obtain:

$$\begin{aligned} \sum_{k' \neq k} \hat{c}_{k'\sigma}^+ \hat{c}_{k\sigma} t_{k'} &= i \sum_{k'} \int^t dt_1 \times \\ &\times [t_{k'}^2 \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma} - t_k t_{k'} \hat{c}_{k'\sigma}^+ \hat{c}_{1\sigma}] \cdot e^{i \cdot (\varepsilon_k - \varepsilon_{k'}) \cdot (t - t_1)}. \end{aligned} \quad (4)$$

Combining Eqs. (4) and (2) we obtain:

$$\begin{aligned} i \frac{\partial \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma}}{\partial t} &+ [\varepsilon_1 - \varepsilon_k + i\Gamma_k] \cdot \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma} + U \hat{n}_{1-\sigma} \cdot \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma} = \\ &= t_k \cdot (\hat{n}_{1\sigma} - \hat{n}_{k\sigma}) + i \sum_{k'} \int^t dt_1 \times \\ &\times t_k t_{k'} \hat{c}_{k'\sigma}^+ \hat{c}_{1\sigma} \cdot e^{i \cdot (\varepsilon_k - \varepsilon_{k'}) \cdot (t - t_1)}, \end{aligned} \quad (5)$$

where $\Gamma_k = \nu_{k0} t_{k(p)}^2$, ν_{k0} - is the unperturbed density of states in the tunneling contact lead. Multiplying Eq. (5) by electron operators $(1 - \hat{n}_{1-\sigma})$ and $\hat{n}_{1-\sigma}$ we obtain the following expressions:

$$\begin{aligned} (1 - \hat{n}_{1-\sigma}) \cdot i \frac{\partial \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma}}{\partial t} &+ [\varepsilon_1 - \varepsilon_k + i\Gamma_k][1 - \hat{n}_{1-\sigma}] \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma} = \\ &= (1 - \hat{n}_{1-\sigma}) \cdot [t_k \cdot (\hat{n}_{1\sigma} - \hat{n}_{k\sigma}) + \\ &+ i \sum_{k'} \int^t dt_1 t_k t_{k'} \hat{c}_{k'\sigma}^+ (t_1) \hat{c}_{1\sigma}(t_1) e^{i \cdot (\varepsilon_k - \varepsilon_{k'}) \cdot (t - t_1)}], \\ \hat{n}_{1-\sigma} \cdot i \frac{\partial \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma}}{\partial t} &+ [\varepsilon_1 - \varepsilon_k + U + i\Gamma_k] \hat{n}_{1-\sigma} \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma} = \\ &= \hat{n}_{1-\sigma} \cdot [t_k \cdot (\hat{n}_{1\sigma} - \hat{n}_{k\sigma}) + \\ &+ i \sum_{k'} \int^t dt_1 t_k t_{k'} \hat{c}_{k'\sigma}^+ (t_1) \hat{c}_{1\sigma}(t_1) e^{i \cdot (\varepsilon_k - \varepsilon_{k'}) \cdot (t - t_1)}]. \end{aligned} \quad (6)$$

If condition $\frac{\varepsilon_1 - \varepsilon_F}{\Gamma} \gg 1$ is fulfilled, $\hat{n}_{1-\sigma}$ is a slowly varying variable in comparison with the $\hat{c}_{1\sigma}^+ \hat{c}_{k\sigma}$ ($\frac{\partial}{\partial t} \hat{n}_{1-\sigma} \ll \frac{\partial}{\partial t} \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma}$). Consequently, it is reasonable to consider that:

$$\frac{\partial}{\partial t} \hat{n}_{1-\sigma} \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma} \sim \hat{n}_{1-\sigma} \frac{\partial}{\partial t} \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma}. \quad (7)$$

So, terms $(\frac{\partial}{\partial t} \hat{n}_{1-\sigma}) \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma}$ are omitted. Omitted terms $\frac{\partial \hat{n}_{1-\sigma}}{\partial t} \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma}$ in the right hand side of Eq. (6) are responsible for the Kondo effect.

One can get expressions for $(1 - \hat{n}_{1-\sigma}) \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma}$ and $\hat{n}_{1-\sigma} \hat{c}_{1\sigma}^+ \hat{c}_{k\sigma}$ (applying the procedure similar to the one which was used to obtain Eq.(4) from Eq.(3)) and then for $\hat{c}_{1\sigma}^+ \hat{c}_{k\sigma}$.

Substituting expression for $\hat{c}_{1\sigma}^+ \hat{c}_{k\sigma}$ to Eq. (2) we obtain equations, which determine time evolution of electron occupation numbers $\hat{n}_{1\sigma}$. It is necessary to note, that the last term in Eq. (5) after summation over index k doesn't contribute to the non-stationary equations for the electron occupation numbers operators are governed by the following system of equations:

$$\begin{aligned} \frac{\hat{n}_{1\sigma}}{\partial t} &= -2\Gamma_k [\hat{n}_{1\sigma} - (1 - \hat{n}_{1-\sigma}) \hat{N}_{k\varepsilon}^\sigma(t) - \hat{n}_{1-\sigma} \hat{N}_{k\varepsilon+U}^\sigma(t)], \\ \frac{\hat{n}_{1-\sigma}}{\partial t} &= -2\Gamma_k [\hat{n}_{1-\sigma} - (1 - \hat{n}_{1\sigma}) \hat{N}_{k\varepsilon}^{-\sigma}(t) - \hat{n}_{1\sigma} \hat{N}_{k\varepsilon+U}^{-\sigma}(t)]. \end{aligned} \quad (8)$$

Before we define $\hat{N}_{k\varepsilon}^\sigma(t)$ and $\hat{N}_{k\varepsilon+U}^\sigma(t)$, one necessary explanation should be made. One can see, that after applying the approximation (7) to Eq.(6) the omitted terms are of the order of Γ_k . It means, that parameter Γ_k in Eq.(6) should be replaced by effective parameter $\Gamma \sim \Gamma_k$.

Operators $\hat{N}_{k\varepsilon}^{\sigma(-\sigma)}(t)$ and $\hat{N}_{k\varepsilon+U}^{\sigma(-\sigma)}(t)$ in Eq.(8) are defined as:

$$\begin{aligned}\hat{N}_{k\varepsilon}^{\sigma}(t) &= \hat{N}_{k\varepsilon}^{-\sigma}(t) = \frac{1}{2}i \int d\varepsilon_k \hat{n}_k^{\sigma}(\varepsilon_k) \times \\ &\times \left[\frac{1 - e^{i(\varepsilon_1 + i\Gamma - \varepsilon_k)t}}{\varepsilon_1 + i\Gamma - \varepsilon_k} - \frac{1 - e^{-i(\varepsilon_1 - i\Gamma - \varepsilon_k)t}}{\varepsilon_1 - i\Gamma - \varepsilon_k} \right], \\ \hat{N}_{k\varepsilon+U}^{\sigma}(t) &= \hat{N}_{k\varepsilon+U}^{-\sigma}(t) = \frac{1}{2}i \int d\varepsilon_k \hat{n}_k^{\sigma}(\varepsilon_k) \times \\ &\times \left[\frac{1 - e^{i(\varepsilon_1 + U + i\Gamma - \varepsilon_k)t}}{\varepsilon_1 + U + i\Gamma - \varepsilon_k} - \frac{1 - e^{-i(\varepsilon_1 + U - i\Gamma - \varepsilon_k)t}}{\varepsilon_1 + U - i\Gamma - \varepsilon_k} \right],\end{aligned}\quad (9)$$

Further we'll consider the situation when the reservoir is paramagnetic: $\hat{N}_{k\varepsilon}^{\sigma}(t) = \hat{N}_{k\varepsilon}^{-\sigma}(t) = \hat{N}_{k\varepsilon}(t)$ and $\hat{N}_{k\varepsilon+U}^{\sigma}(t) = \hat{N}_{k\varepsilon+U}^{-\sigma}(t) = \hat{N}_{k\varepsilon+U}(t)$. We can obtain equations for the occupation numbers of localized electrons $n_{1\pm\sigma}$ by averaging Eqs. (8)-(9) for the operators and by decoupling electrons occupation numbers in the reservoir. Such decoupling procedure is reasonable if one considers that electrons in the macroscopic reservoir is in the thermal equilibrium. After decoupling one has to replace electron occupation numbers operators in the reservoir \hat{n}_k^{σ} by the Fermi distribution functions f_k^{σ} in Eqs. (5)-(9).

We'll investigate time dependent dynamics of the electron occupation numbers and their correlation functions for the different initial conditions: 1) the non-zero localized magnetic moment exists on the impurity ($|n_{1\sigma} - n_{1-\sigma}| \sim 1$). Such state can be prepared due to the applied external magnetic field $\mu B \gg \varepsilon_1$, which is switched "off" at the initial time moment $t = 0$; 2) the initial state close to highly occupied paramagnetic one ($|1 - n_{1\pm\sigma}| \ll 1$) can be prepared by the applied bias voltage $|eV| > \varepsilon_1 + U$ switching "off" or "on" at the initial time moment $t = 0$; 3) the initial state close to the low occupied paramagnetic one ($|n_{1\pm\sigma}| \ll 1$) can be prepared by the applied bias voltage $|eV| < \varepsilon_1$ switching "off" or "on" at the initial time moment $t = 0$. It will be shown that relaxation time scale strongly depends on the properties of the initially prepared state. The solution of kinetic equations (8) for electron occupation numbers $n_{\pm\sigma}$ can be easily found numerically for the arbitrary initial conditions.

If one is interested in the system evolution for the time scales $t \gg \frac{1}{\varepsilon_1}$, fast oscillating terms, which contain time dependent exponents can be neglected. Consequently, functions $N_{k\varepsilon}$ and $N_{k\varepsilon+U}$ become time-independent. So, localized electrons occupation numbers $n_{1\sigma}$, $n_{1-\sigma}$ satisfy the linear system of equations, which can be easily solved for the arbitrary initial conditions:

$$\begin{aligned}n_{1\sigma} &= \frac{N_{k\varepsilon}}{1 + \Delta N} \cdot (1 - e^{\lambda_2 t}) + \\ &+ \frac{n_{1\sigma}(0) - n_{1-\sigma}(0)}{2} \cdot e^{\lambda_1 t} + \frac{n_{1\sigma}(0) + n_{1-\sigma}(0)}{2} \cdot e^{\lambda_2 t}, \\ n_{1-\sigma} &= \frac{N_{k\varepsilon}}{1 + \Delta N} \cdot (1 - e^{\lambda_2 t}) + \\ &+ \frac{n_{1-\sigma}(0) - n_{1\sigma}(0)}{2} \cdot e^{\lambda_1 t} + \frac{n_{1-\sigma}(0) + n_{1\sigma}(0)}{2} \cdot e^{\lambda_2 t}.\end{aligned}\quad (10)$$

The eigenvalues $\lambda_{1,2}$ are determined as:

$$\lambda_{1,2} = -2\Gamma \cdot (1 \mp \Delta N) \quad (11)$$

and

$$\Delta N = N_{k\varepsilon} - N_{k\varepsilon+U}. \quad (12)$$

Straightforward calculations yield:

$$\begin{aligned}\Delta N &= \frac{1}{\pi} [\arctan(-\frac{\varepsilon_1}{\Gamma}) - \arctan(\frac{-\varepsilon_1 + W}{\Gamma}) - \\ &- \arctan(-\frac{\varepsilon_1 + U}{\Gamma}) + \arctan(\frac{W - (\varepsilon_1 + U)}{\Gamma})].\end{aligned}\quad (13)$$

where W - is a band width for the conduction electrons in the reservoir.

In the case of the large bandwidth for $\varepsilon_1 < 0$, $\varepsilon_1 + U > 0$, $|\varepsilon_1|/\Gamma \gg 1$ and $(\varepsilon_1 + U)/\Gamma \gg 1$ one can obtain:

$$\begin{aligned}\frac{|\lambda_1|}{2\Gamma} &\sim \frac{\Gamma U}{2|\varepsilon_1|(U - |\varepsilon_1|)}, \\ \frac{|\lambda_2|}{2\Gamma} &\sim 2 - \frac{\Gamma U}{2|\varepsilon_1|(U - |\varepsilon_1|)}.\end{aligned}\quad (14)$$

For the large values of Coulomb interaction and deep energy level of the localized state, relaxation time $|\lambda_1|^{-1}$ can be several orders larger than the relaxation time of initial localized state in the absence of Coulomb interaction. Relaxation rates behavior for the different system parameters is shown in Fig.1 and Fig.2. Relaxation rates for the magnetic moment and charge strongly differ for the deep energy levels (see Fig.1), but they nearly become equal for the energy levels $\varepsilon_1 > 0$ or $\varepsilon_1 + U < 0$. The role of Coulomb correlations was also analyzed (see Fig.2). The presence of Coulomb correlations results in the increasing of the relaxation values difference.

Typical time for the system to achieve the stationary state depends on the initial conditions. For the "paramagnetic" initial conditions ($n_{1\sigma}(0) = n_{1-\sigma}(0)$) relaxation rate to the stationary state is determined by $|\lambda_2| = 2\Gamma \cdot (1 + \Delta N)$ and in the case of the "magnetic" initial conditions ($|n_{1\sigma}(0) - n_{1-\sigma}(0)| \sim 1$) relaxation rate to

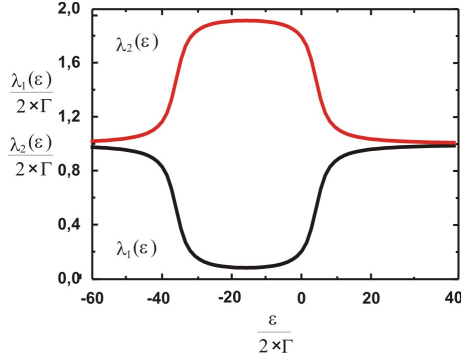


FIG. 1. (Color online) Normalized relaxation rates $|\lambda_{1,2}(\varepsilon)|/2\Gamma$ as a functions of the localized state energy level position $\varepsilon/2\Gamma$ for $U/2\Gamma = 7.5$ and $\Gamma = 1$.

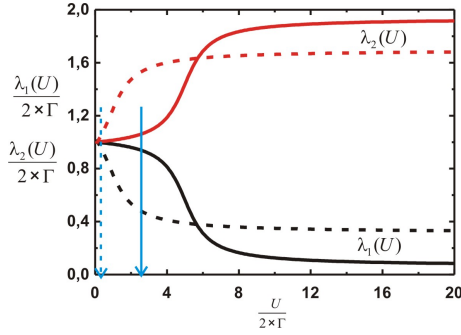


FIG. 2. (Color online) Normalized relaxation rates $|\lambda_{1,2}(U)|/2\Gamma$ as a functions of Coulomb interaction value $U/2\Gamma$ for $\Gamma = 1$. Blue arrows demonstrate localized states energy levels values. Solid lines $|\varepsilon|/2\Gamma = 2.5$; dashed lines $|\varepsilon|/2\Gamma = 0.375$.

the stationary state is determined by $|\lambda_1| = 2\Gamma \cdot (1 - \Delta N)$. Consequently, we have long living "magnetic" moments.

In the presence of interaction with the "paramagnetic" reservoir ($\Gamma \neq 0$) stationary state is always a "paramagnetic" one:

$$n_1^{st} = n_{1\sigma} = n_{1-\sigma} = \frac{N_{k\varepsilon}}{1 + \Delta N}. \quad (15)$$

The behavior of localized state electron occupation numbers for the different initial conditions and the set of system parameters is depicted in Fig.(4)-Fig.(5). Panels a,c correspond to the case when Coulomb interaction is present and panels b,d - describe the situation when relaxation takes place in the absence of Coulomb correlations. Magnetic properties are revealed for $|\varepsilon_1| < 0$, $\varepsilon_1 + U > 0$, $|\varepsilon_1|/\Gamma \gg 1$ and $(\varepsilon_1 + U)/\Gamma \gg 1$ in the slow relaxation of the initial "magnetic" state, prepared at $t = t_0$ ($|\lambda_1| \ll |\lambda_2|$) (see Fig.4). Nonzero magnetic moment is present on the impurity for $t \gg (2\Gamma)^{-1}$. So, the time scale when magnetic moment exists on the impurity (see panel a,c in Fig.(4)-Fig.(5)) strongly exceeds the relaxation time for the impurity state without Coulomb interaction (see panel b,d in Fig.(4)-Fig.(5)). Obtained

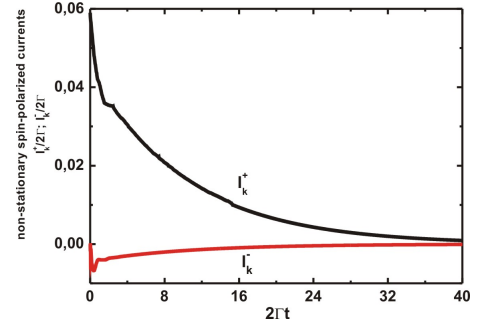


FIG. 3. (Color online) Normalized non-stationary spin-polarized tunneling currents $I^+(t)/2\Gamma$ (black line) and $I^-(t)/2\Gamma$ (red line). $n_{1\sigma}(0) = 1$ and $n_{1-\sigma}(0) = 0$; $\varepsilon/2\Gamma = -2.5$; $U/2\Gamma = 7.5$ and $\Gamma = 1$.

results demonstrate, that the stationary state of the single impurity with Coulomb correlations in the presence of interaction with the reservoir is always "paramagnetic". The mean values of the electron occupation numbers with the opposite spin directions in the stationary case have the same magnitudes for any value of the on-site Coulomb repulsion, contrary to the results obtained in the mean-field approximation.

We revealed that typical times of the stationary state formation are determined by the initial conditions. For the deep energy levels and strong Coulomb correlations (see panels a in the Fig.(4)-Fig.(5)), relaxation time for the initial "magnetic" state can be several orders larger than for the "paramagnetic" one. This fact reflects the "magnetic" nature of the single occupied localized state with strong Coulomb correlations. The presence of long-living "magnetic" moment depends on the ratio between the system parameters: the single electron level position, the value of Coulomb interaction and coupling to reservoir.

Non-stationary spin polarized currents flowing in opposite directions for different spins exists in the system in the particular time interval (see Fig.4). Non-stationary spin-polarized tunneling currents are determined by the right-hand side of Eq. (8). For $|\lambda_1|^{-1} > t > (2 \cdot \Gamma)^{-1}$:

$$\frac{1}{e} \cdot I^\pm = \frac{\partial n_{1\pm\sigma}}{\partial t} \sim \pm [n_{1\sigma}(0) - n_{1-\sigma}(0)] \cdot \lambda_1 \cdot e^{\lambda_1 t}. \quad (16)$$

For typical $\Gamma \sim 1 \div 10$ meV and $|\varepsilon| \sim 50$ meV, corresponding to the situation depicted in Fig.3 the non-stationary spin-polarized current value is about $1 \div 10$ nA ($1\text{ nA} \simeq 6 \times 10^9 e/\text{sec}$).

Charge transfer by the electrons with the "up" and "down" spins is determined as:

$$\frac{1}{e} \cdot \Delta Q^\pm = n_{1\pm\sigma}(0) - \frac{N_{k\varepsilon}}{1 + \Delta N}. \quad (17)$$

For $n_{1\sigma}(0) - n_{1-\sigma}(0) \sim 1$ and deep energy levels in the presence of strong Coulomb interaction:

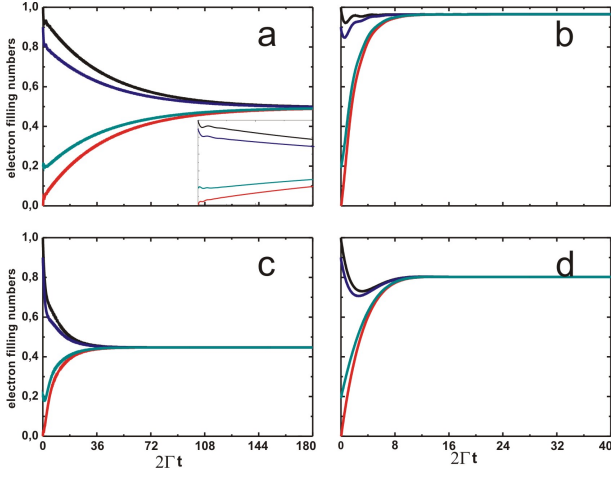


FIG. 4. (Color online) Electron occupation numbers time evolution for the "magnetic" initial conditions. Black and blue lines demonstrate $n_{1\sigma}(t)$, red and green lines - $n_{1-\sigma}(t)$. a),b) $\varepsilon/2\Gamma = -2.5$; c),d) $\varepsilon/2\Gamma = -0.375$. a),c). long-living "magnetic" moments in the presence of Coulomb interaction $U/2\Gamma = 7.5$; b),d). fast relaxation in the absence of Coulomb interaction $U/2\Gamma = 0$. Parameter $\Gamma = 1$ is the same for all the figures. Black line - $n_{1\sigma}(0) = 1$, red line - $n_{1-\sigma}(0) = 0$, blue line - $n_{1\sigma}(0) = 0.9$, green line - $n_{1-\sigma}(0) = 0.2$. Insert demonstrates the presence of oscillations at the very beginning of charge relaxation.

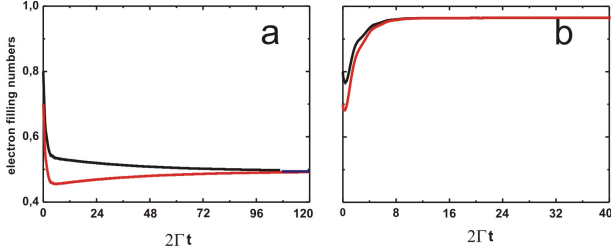


FIG. 5. (Color online) The absence of large time scale in electron occupation numbers time evolution for the initial conditions close to the "paramagnetic" one. Black line demonstrates $n_{1\sigma}(t)$, red line - $n_{1-\sigma}(t)$. a). in the presence of Coulomb interaction $U/2\Gamma = 7.5$; b). in the absence of Coulomb interaction $U/2\Gamma = 0$. Parameters $\varepsilon/2\Gamma = -2, 5$ and $\Gamma = 1$ are the same for all the figures. Black line $n_{1\sigma}(0) = 0.8$, red line $n_{1-\sigma}(0) = 0.7$.

$$|\Delta Q^+| - |\Delta Q^-| \sim \frac{\Gamma}{4\varepsilon_1}. \quad (18)$$

So, the total non-stationary charge transfer is connected with the particular spin electrons, but it's value is small for $\Gamma/\varepsilon_1 < 1$. This situation resembles the spin-Hall systems with two types of "edge" states with the opposite velocities and spins at each system boundary with negligible charge transfer from the one boundary to the another²².

If impurity energy level is localized above the Fermi level E_F , two time scales $|\lambda_1|^{-1}$ and $|\lambda_2|^{-1}$ are of the

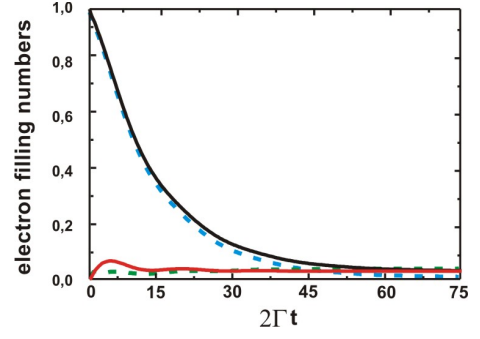


FIG. 6. (Color online) Electron occupation numbers time evolution for $\varepsilon/2\Gamma = 2.5$, $\Gamma = 1$. Black solid and blue dashed lines demonstrate $n_{1\sigma}(t)$, red solid line and green dashed lines - $n_{1-\sigma}(t)$. Solid lines $U/2\Gamma = 7.5$, dashed lines $U/2\Gamma = 0$.

same order even for strong Coulomb interaction and for magnetic initial conditions (see Fig.6).

The magnetic properties can be also analyzed from the time dependence of the stationary correlation functions for the electron occupation numbers:

$$K^{\sigma\sigma'}(t-t') = \langle n_{1\sigma}(t)n_{1\sigma'}(t') \rangle. \quad (19)$$

Correlation functions $K^{\sigma\sigma'}(\tau = t - t')$ satisfy the system of equations, which is derived from Eq.(8) for electron occupation numbers:

$$\begin{aligned} \frac{\partial}{\partial t} K^{+-} &= -2\Gamma_k [K^{+-} + \Delta N K^{--} - N_{k\varepsilon} n_{1-\sigma}], \\ \frac{\partial}{\partial t} K^{--} &= -2\Gamma_k [K^{--} + \Delta N K^{+-} - N_{k\varepsilon} n_{1-\sigma}]. \end{aligned} \quad (20)$$

Initial conditions are determined as:

$$\begin{aligned} K^{+-}(t, t) &= K^{+-}(0) = \frac{N_{k\varepsilon+U} \cdot N_{k\varepsilon}}{1 + \Delta N} \\ K^{--}(0) &= n_1^{st} = \frac{N_{k\varepsilon}}{1 + \Delta N}. \end{aligned} \quad (21)$$

Time evolution of the correlation functions can be obtained from the Eq. (20):

$$\begin{aligned} K^{+-}(\tau) &= \frac{N_{k\varepsilon}^2}{(1 + \Delta N)^2} \cdot [1 - e^{\lambda_2 \tau}] + \\ &+ \frac{N_{k\varepsilon} [N_{k\varepsilon+U} - 1]}{2[1 + \Delta N]} \cdot e^{\lambda_1 \tau} + \frac{N_{k\varepsilon} [N_{k\varepsilon+U} + 1]}{2[1 + \Delta N]} \cdot e^{\lambda_2 \tau}, \\ K^{--}(\tau) &= \frac{N_{k\varepsilon}^2}{(1 + \Delta N)^2} \cdot [1 - e^{\lambda_2 \tau}] + \\ &+ \frac{N_{k\varepsilon} [N_{k\varepsilon+U} + 1]}{2[1 + \Delta N]} \cdot e^{\lambda_2 \tau} + \frac{N_{k\varepsilon} [1 - N_{k\varepsilon+U}]}{2[1 + \Delta N]} \cdot e^{\lambda_1 \tau}. \end{aligned} \quad (22)$$

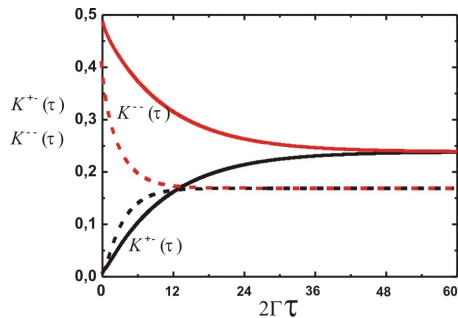


FIG. 7. (Color online) Correlation functions time evolution for the "magnetic" initial conditions. Black lines demonstrate K_{τ}^{+-} , red lines - K_{τ}^{--} . Solid lines $\varepsilon/2\Gamma = -2.5$; Dashed lines $\varepsilon/2\Gamma = -0.375$. Parameters $U/2\Gamma = 7.5$ and $\Gamma = 1$.

The behavior of the stationary correlation functions for the localized electrons occupation numbers with the different spin orientation is depicted in Fig.7. It is clearly evident, that for the deep energy levels correlation functions time evolution is much lower, than for the states with shallow energy levels. Autocorrelation function for the electron occupation numbers with the opposite spins tends to zero for the strong Coulomb interaction. Such behavior points to the possibility of the presence of non-zero magnetic moment in a certain time interval.

For $\tau \rightarrow \infty$ correlation functions turns to the product of the decoupled electronic occupation numbers mean values:

$$K^{+-st} = K^{--st} \simeq \left(\frac{N_{k\varepsilon}}{1 + \Delta} \right). \quad (23)$$

So for $\tau < \frac{1}{|\lambda_1|}$ the "magnetic" correlations are still present in the system. Time evolution of $K^{+-}(\tau)$ and $K^{--}(\tau)$ is depicted in Fig.7.

III. CONCLUSION

We demonstrated that the difference between "magnetic" and "paramagnetic" states in the single-impurity Anderson model appears only in the non-stationary characteristics of the system and in the second order correlation functions behavior. Localized

state dynamics in the presence of interaction with the reservoir and Coulomb correlations has been analyzed by means of the kinetic equations for the electron occupation numbers with the different spins, taking into account high order correlation functions for the localized electrons.

We revealed that the stationary state of the single impurity with Coulomb correlations in the presence of interaction with the reservoir is always a "paramagnetic" one, even when interaction is weak. Electron occupation numbers with the opposite spin in the stationary case have are equal for any value of the on-site Coulomb repulsion, contrary to the results obtained in the mean-field approximation. To reveal "magnetic" properties for the single-impurity Anderson model one has to analyze non-stationary system characteristics.

We showed that typical times of the stationary state formation depend on the initial conditions. For the deep energy levels and strong Coulomb correlations, relaxation time for the initial "magnetic" state can be several orders larger than for the "paramagnetic" one. This fact reflects the "magnetic" nature of the single occupied localized state with the strong Coulomb correlations. Described relaxation times difference allows to distinguish the "magnetic" state on the localized impurity from the "paramagnetic" one. The existence of long-living "magnetic" moment depends on the ratio between the system parameters: the single electron level position, the value of Coulomb interaction and coupling to reservoir.

We analyzed the behavior of the correlation functions for the localized electrons occupation numbers with the different spin orientation. For the large time scales, which can strongly exceed relaxation time of the system in the absence of Coulomb interaction, rather strong correlations of the electron occupation numbers are present. Such behavior of correlation functions points to the existence of magnetic regime.

For initially magnetic impurities non-stationary spin polarized currents flowing in the opposite directions for the different spins exist in the system in the particular time interval similar to the spin-Hall systems with the two types of the "edge" states with opposite velocities and spins at each boundary.

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